

CLAIMS

1. A computer system comprising a database having a plurality of records, wherein each record comprises a field point representation representing field extrema
5 for a conformation of a chemical structure.
2. The computer system of claim 1, wherein the database includes records for multiple conformations of the same chemical structure.
- 10 3. The computer system of claim 1 or 2, wherein each record further comprises a structural representation of the chemical structure.
4. The computer system of any preceding claim, each record having an index of the field point representation, wherein the index is a searchable representation of the
15 field point representation.
5. The computer system of claim 4, wherein the index is a string.
6. The computer system of claim 4 or 5, each record having multiple indexes of the field point representation, wherein the multiple indexes are representations of the field point representation at different precision levels.
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7. The computer system of claim 4, 5 or 6, comprising an indexing mechanism for generating an index of a field point representation.
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8. The computer system of claim 7, wherein an index is a string of length n and the indexing mechanism is configured to:
 - (i) generate a numeric identifier from a characteristic of the field point representation;

- (ii) generate one or more numbers in a range from 1 to n in dependence on the numeric identifier;
 - (iii) increment the bins in the string that correspond to the one or more numbers;
and
- 5 (iv) optionally repeat (i) to (iii) for another characteristic of the field point representation.

9. The computer system of claim 8, wherein a characteristic of the field point representation includes one or more of:

- 10 the number of field points of a particular field of the field point representation;
the particular field and energy of a field point in the field point representation;
and
the respective energies of and distance between a field point pairing in the field point representation.

- 15 10. The computer system of claim 8 or 9, wherein the indexing mechanism is configured to take a measurement of a characteristic of the field point representation to generate the numeric identifier.

- 20 11. The computer system of claim 10, wherein the indexing mechanism is configured to take a measurement of the characteristic of the field point representation at different levels of precision to generate corresponding multiple indexes which represent the field point representation at different precision levels.

- 25 12. The computer system of any of claims 8, 9, 10 or 11, wherein the indexing mechanism is configured to:
 - (i) define a plurality of ranges of possible measurement values;
 - (ii) take a measurement of a characteristic of the field point representation to produce a measurement value;

- (iii) assign the measurement value to a range if the measurement value is within the range;
 - (iv) optionally repeat (ii) and (iii); and
 - (v) use the number of measurement values assigned to the range to generate the numeric identifier.
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13. The computer system of claim 12, wherein the indexing mechanism is configured to define ranges of equal width across all ranges.
- 10 14. The computer system of claim 12, wherein the indexing mechanism is configured to define a range for smaller measurement values with a narrower width than a range for larger measurement values.
- 15 15. The computer system of any of claims 12, 13 or 14, wherein the indexing mechanism is configured to generate multiple indexes by defining ranges of different widths for different precision levels.
- 20 16. The computer system of any of claims 8 to 15, wherein the indexing mechanism is configured to generate one or more numbers in a range from 1 to n in dependence on the numeric identifier by using a deterministic function.
17. The computer system of claim 16, wherein the deterministic function is a pseudo-random number generator or a hash function.
- 25 18. The computer system of any one of claims 8 to 17, wherein the bins in the string take real number values.
19. The computer system of claim 18, wherein the real number value is generated from the energies of a pair of field points in the field point representation.

20. The computer system of any preceding claim, comprising a searching mechanism for searching the database.

21. The computer system of claim 20, wherein the searching mechanism is
5 configured to:

- (i) compare a query index with an index of a field point representation for a record in the database;
- (ii) identify the record as a hit if the comparison satisfies a search criterion; and
- (iii) repeat (i) and (ii) for a plurality of records.

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22. The computer system of claim 21, wherein the searching mechanism is further configured to:

receive a search query identifying a field point representation;
form the query index by generating an index of the field point representation
15 identified by the search query.

23. The computer system of any of claims 20 to 22, wherein the search mechanism is configured to search by precision level.

20 24. A database for implementation on a computer system, the database configured to support a plurality of records, each record comprising a field point representation representing field extrema for a conformation of a chemical structure.

25 25. The database of claim 24, configured to support each record having an index of the field point representation, wherein the index is a searchable representation of the field point representation.

26. The database of claim 25, wherein the index is a string.

27. The database of any of claims 24 to 26, configured to support each record having multiple indexes of the field point representation, wherein the multiple indexes are representations of the field point representation at different precision levels.
- 5 28. The database of any of claims 24 to 27, comprising an indexing mechanism for generating an index of a field point representation.
29. The database of any of claims 24 to 28, comprising a searching mechanism for searching the database.
- 10 30. Computer software configured to provide the database of any of claims 24 to 29.
- 15 31. A carrier medium carrying computer software configured to provide the database of any of claims 24 to 29.
32. A method of generating an index of a field point representation representing field extrema for a conformation of a chemical structure, wherein the index is a string with n elements, the method comprising:
- 20 (i) generating a numeric identifier from a characteristic of the field point representation;
- (ii) generating one or more numbers in a range from 1 to n in dependence on the numeric identifier;
- (iii) incrementing the string elements that correspond to the one or more numbers;
- 25 and
- (iv) optionally repeating (i) to (iii) for another characteristic of the field point representation.
33. The method of claim 32, comprising taking a measurement of a characteristic of the field point representation to generate the numeric identifier.

34. The method of claim 33, comprising taking the measurement of the characteristic of the field point representations at different levels of precision to generate corresponding multiple indexes which represent the field point representation
5 at different precision levels.
35. The method of any of claims 32 to 34, comprising
(i) defining a plurality of ranges of possible measurement values;
(ii) taking a measurement of a characteristic of the field point representation to
10 produce a measurement value;
(iii) assigning the measurement value to a range if the measurement value is within the range;
(iv) optionally repressing (ii) and (iii); and
(v) using the number of measurement values assigned to a range to generate the
15 numeric identifier.
36. The method of claim 35, comprising defining ranges of equal width across all ranges
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37. The method of claim 35, comprising defining a range for smaller measurement values with a narrower width than a range for larger measurement values.
38. The method of any of claims 35, 36 or 37, comprising generating multiple indexes by defining ranges of different widths for different precision levels.
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39. The method of any of claims 32 to 38, comprising using a deterministic function to generate one or more numbers in a range from 1 to n in dependence on the numeric identifier.

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40. The method of claim 39, wherein the deterministic function is a pseudo-random number generator or a hash function.

41. A method of searching a database having a plurality of records, each record comprising a field point representation representing field extrema for a conformation of a chemical structure and having an index of the field point representation, the method comprising:
- (i) comparing a query index with an index of a field point representation for a record in the database;
 - 10 (ii) identifying the record as a hit if the comparison satisfies a search criterion;
 - (iii) repeating (i) and (ii) for a plurality of records; and
 - (iv) outputting a representation of the records identified as a hit.

42. The method of claim 41, further comprising:

- 15 receiving a search query identifying a field point representation; and
forming the query index by generating an index of the field point representation identified by the search query.

43. The method of claim 41 or 42, the method further comprising searching by
20 precision level.